Pis'ma v ZhETF, vol. 74, iss. 12, pp. 674 – 677 © 2001 December 25

The Berezinskii–Kosterlitz–Thouless transition and correlations in the XY kagomé antiferromagnet

*V. B. Cherepanov, I. V. Kolokolov+, E. V. Podivilov**

Hummingberg Ltd., Toronto, Ontario, Canada M2H 2S6,

+Budker Institute of Nuclear Physics, 630090 Novosibirsk, Russia

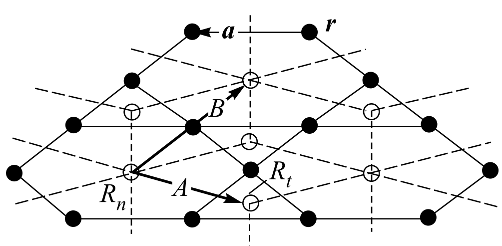
**Institute of Automation and Electrometry RAS, 630090 Novosibirsk, Russia*

Submitted 20 November 2001

The problem of the Berezinskii-Kosterlitz-Thouless transition in the highly frustrated XY kagomé antiferromagnet is solved. The transition temperature is found. It is shown that the spin correlation function exponentially decays with distance even in the low-temperature phase, in contrast to the order parameter correlation function, which decays algebraically with distance.

PACS: 74.50.+r, 75.10.Hk, 75.50.Ee

Generally, XY spins on two-dimensional lattices undergo a Berezinskii-Kosterlitz-Thouless (BKT) transition [1, 2]. If there is no frustration, physics of this transition does not depend on details of lattice structure. At finite temperatures the behaviour of a system is governed by spin waves and vortices. They are well defined in continuum limit of the theory. In the low-temperature phase the spin vortices are bound in pairs with zero topological charge and spin correlators decay with distance algebraically. One can define also vorticity field demonstrating non-trivial dynamical correlations [3]. In the BKT transition point the vortex-antivortex interaction becomes screened, pairs disintegrate and the spin correlation length turns to be finite. By contrast, the XY antiferromagnet on the two-dimensional kagomé lattice (see Figure) has infinitely many ground states, and its description in terms of continuous field theory is not justified.



The kagomé lattice (filled dots) with antiferromagnetic bonds (continuous lines) and the dual lattice (circles) and its bonds (dashed lines)

In the present paper we compute BKT transition temperature in this systems. In [4] it was suggested that the true order parameter here is $\eta = e^{3i\theta}$ where θ is the angle of a spin. It is invariant with respect to any arbitrary choice of ground states, which are a subset of local $2\pi/3$ spin rotations. Therefore this order parameter can change smoothly in the plane. The phase transition consists in the emergence of finite correlation length of the variable η. Its indirect evidence was obtained from Monte-Carlo simulations in [5, 6]. As for the correlation length of spins itself, we show here that it is finite starting from arbitrary small temperature. It is inevitable consequence of finite values of energy barriers separating different vacua.

In order to take into account the special structure of the kagomé lattice we start with the approach developed in [7] (see also [8]). The kagomé lattice consists of triangles and hexagons (Figure). The Hamiltonian of the kagomé antiferromagnet can be represented as a sum of squares of the total spins $\mathbf{S}_t$ in triangles $\{t\}$ of the nearest neighbors:

$$H = \frac{\kappa}{2}\sum_t \left(\mathbf{S}_t\right)^2 . \qquad (1)$$

Each spin participates in two triangles. The ground state energy is equal to zero and there are infinitely many ground states with $\mathbf{S}_t = 0$. In any ground state, the angles between neighboring spins are equal to $\pm 2\pi/3$.

The partition function of the XY kagomé antiferromagnet can be represented as an integral of a function defined on the lattice's bonds:

$$Z(\beta) = \int \exp\left(-\beta\sum_{\mathbf{r},\mathbf{a}}\cos\Theta_{\mathbf{r},\mathbf{a}}\right)\prod_{\mathbf{r}} d\theta(\mathbf{r}), \qquad (2)$$
$$\Theta_{\mathbf{r},\mathbf{a}} \equiv \theta(\mathbf{r}+\mathbf{a}) - \theta(\mathbf{r}),$$

where $\mathbf{r}$ marks positions on the kagomé lattice, $\mathbf{a}$ are the three lattice vectors directed along the antiferromagnetic bonds between nearest neighbors, $\theta_{\mathbf{r}}$ are the spin angles, and $\beta = \kappa S^2/2T$ is the dimensionless inverse temperature. The 2π periodicity of the angle variables allows one to expand the statistical weight in (2) in Fourier series with the coefficients $I_{n(\mathbf{r},\mathbf{a})}(-\beta)$:

$$\exp\left(-\beta \sum\nolimits_{\mathbf{r},\mathbf{a}} \cos\Theta_{\mathbf{r},\mathbf{a}}\right) = \\ = \prod\nolimits_{(\mathbf{r},\mathbf{a})} \sum\nolimits_{n(\mathbf{r},\mathbf{a})} I_{n(\mathbf{r},\mathbf{a})}(-\beta) \exp\left(in(\mathbf{r},\mathbf{a})\Theta_{\mathbf{r},\mathbf{a}}\right). \quad (3)$$

Here $I_n(x)$ is the modified Bessel function and integer numbers $n(\mathbf{r},\mathbf{a})$ are located on bonds connecting nearest neighbors $\mathbf{r}$ and $\mathbf{r}+\mathbf{a}$. Then we integrate over the angles $\theta(\mathbf{r})$ and arrive to the following representation for the partition function:

$$Z(\beta) = \sum_{\{n(\mathbf{r},\mathbf{a})\}} \prod_{\mathbf{r}} \Delta\left(\sum_{\mathbf{a}} n(\mathbf{r},\mathbf{a})\right) \prod_{\mathbf{a}} I_{n(\mathbf{r},\mathbf{a})}(-\beta), \quad (4)$$

where $n(\mathbf{r}+\mathbf{a},-\mathbf{a}) = -n(\mathbf{r},\mathbf{a})$. Here $\{n(\mathbf{r},\mathbf{a})\}$ denotes the set of all the configurations of integers $n(\mathbf{r},\mathbf{a})$. The Δ-function ($\Delta(0) = 1$, $\Delta(n \neq 0) = 0$) expresses the conservation condition at each site of the lattice:

$$\sum_{\mathbf{a}} n(\mathbf{r},\mathbf{a}) = 0. \quad (5)$$

As in the case of perturbation theory graphs [9], this means that the summation in (4) runs effectively over integer-valued currents $J(\mathbf{R})$ circulating in closed loops. The latter are numbered by dual lattice sites $\mathbf{R}_t$ and $\mathbf{R}_h$ which are located in centers of triangles and hexagons correspondingly (Figure). A current $n(\mathbf{r},\mathbf{a})$ along a bond is equal to the sum of currents in one triangle and in one hexagon that share the bond $(\mathbf{r},\mathbf{a})$. This allows us to represent the partition function as follows:

$$Z(\beta) = \sum_{\{J(\mathbf{R}_h)\}} \prod_{\mathbf{R}_t} \sum_{J(\mathbf{R}_t)} \prod_{h=1}^{3} I_{J(\mathbf{R}_t+\mathbf{A}_h)+J(\mathbf{R}_t)}(-\beta). \quad (6)$$

Here we separate the sums over triangle and hexagon currents, $J(\mathbf{R}_t)$ and $J(\mathbf{R}_h)$, with centers $\mathbf{R}_t$ and $\mathbf{R}_h = \mathbf{R}_t + \mathbf{A}_h$, and h numbers three hexagons surrounding each triangle $\mathbf{R}_t$. Further on, we consider $e^{-\beta}$ as a small parameter of the theory. We will see that the inequality $e^{-\beta} \ll 1$ holds even in the BKT transition point as for the square lattice [1, 2, 7]. However, the Bessel functions in Eq. (6) cannot be substituted by their asymptotics at $\beta \gg 1$ because the summation over $J(\mathbf{R}_t)$ results in relatively small contribution to $Z(\beta)$. This asymptotic corresponds to saturation of maximal number of nearest neighbors' bounds, what is far away from the true ground state due to frustrations. Consequently, the summation over the triangle currents $J(\mathbf{R}_t)$ must be performed first. To do this we represent triple products of the Bessel functions in (6) in the integral form, what allows us to take the sum over $J(\mathbf{R}_t)$ exactly:

$$\sum_{J(\mathbf{R}_t)} \prod_{h=1}^{3} I_{J(\mathbf{R}_t+\mathbf{A}_h)+J(\mathbf{R}_t)}(-\beta) = \\ = \sum_{m=-1,0,1} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \frac{d\phi_1 d\phi_2 d\phi_3}{(2\pi)^3} \times \\ \times \delta\left(\phi_1+\phi_2+\phi_3+2\pi m\right) \times \\ \times \exp\left[-\sum_{h=1}^{3} i\phi_h J(\mathbf{R}_t+\mathbf{A}_h) + \beta\cos(\phi_h)\right] \sim \\ \sim \sum_{\sigma(\mathbf{R}_t)=\pm 1} \exp\left\{\frac{i2\pi\sigma(\mathbf{R}_t)}{3}\sum_{h=1}^{3} J(\mathbf{R}_h) - \right. \\ \left. - \frac{1}{6\beta}\sum_{h',h=1}^{3}\left(J(\mathbf{R}_{h'}) - J(\mathbf{R}_h)\right)^2\right\}. \quad (7)$$

Here $\mathbf{R}_h = \mathbf{R}_t + \mathbf{A}_h$ for a given t. The last asymptotic relation in (7) follows from that the integration over $d\phi_1 d\phi_2 d\phi_3$ at large β is saturated by vicinity of two saddle points $\phi_h = 2\pi\sigma(\mathbf{R}_t)/3$, where $\sigma(\mathbf{R}_t) = \pm 1$ ($h = 1,2,3$). Thus, hexagon currents and chiralities $\sigma = \pm 1$ residing in triangles remain. These variables count the multiple ground states. Substituting the asymptotic formula for the triple products of Bessel functions (7) into (6) and using the Poisson summation formula we arrive at the following expression for the partition function:

$$Z(\beta) = \sum_{\{\sigma(\mathbf{R}_t)\},\{m(\mathbf{R}_h)\}} \int \exp\left\{2\pi i \sum_{\mathbf{R}_h} J(\mathbf{R}_h) Q(\mathbf{R}_h) - \right. \\ \left. - \frac{1}{3\beta}\sum_{\mathbf{R}_h,\mathbf{B}_h}\left(J(\mathbf{R}_h) - J(\mathbf{R}_h+\mathbf{B}_h)\right)^2\right\} \prod_{\mathbf{R}_h} \mathrm{d}J(\mathbf{R}_h), \quad (8)$$

$$Q(\mathbf{R}_h) = m(\mathbf{R}_h) + \frac{1}{3}\sum_{\mathbf{A}_t}\sigma(\mathbf{R}_h+\mathbf{A}_t). \quad (9)$$

Here $\mathbf{A}_t$ runs over all six triangles surrounding each hexagon with the centers $\mathbf{R}_h$, $\mathbf{R}_t = \mathbf{R}_h + \mathbf{A}_t$, and $\mathbf{B}_h$ are six vectors that connect the centers of nearest hexagons. Note that centers of hexagons form a triangular lattice which is dual to the hexagonal lattice.

Now one can integrate the partition function (8) over the currents in hexagons, $J(\mathbf{R}_h)$. This results in the expression for the partition function of the 2D Coulomb gas with charges $Q(\mathbf{R}_h)$ positioned on sites of the triangular lattice $\mathbf{R}_h$. Charges are 1/3-multiple, this corresponds to the $2\pi/3$-multiplicity of vortex rotations. At zero temperature, the integration over $J(\mathbf{R}_h)$ in (8) yields conservation conditions $\prod_{\mathbf{R}_h} \delta(Q(\mathbf{R}_h))$, i. e., in any ground state, the sum of chiralities of triangles surrounding each hexagon is a multiple of 3. The problem of counting ground states is mapped onto that of coloring of the hexagonal lattice [4] which was solved exactly [10]. The exact number of ground states, Z_N, is equal to $1.46099^{N/3}$, where N is the number of spins. A naive approximation that assumes that chiralities of triangles surrounding each hexagon are independent and equally probable gives a good estimate $Z_N \approx (11/8)^{N/3} = 1.375^{N/3}$ for the number of the ground states. In this estimate we neglect correlations between chiralities of triangles surrounding neighboring hexagons. Their effect can be estimated as the inverse number of the nearest neighbors on the triangular lattice, 1/6. At finite temperatures we divide $J(\mathbf{R})$ into slowly varying and short wavelength fields and integrate first over the latter. This gives product of local statistical weights $\prod_n \exp\left(-3\beta\pi^2 Q_n^2/8\right)$ which substitutes the product of δ-functions at $\beta \to \infty$. The BKT transition point is determined by exitations with most probable charges: $Q_n = 0, \pm 1/3$. States with the sum of chiralities of triangles surrounding a certain hexagon equal to ± 2 and ± 4 contribute to formation of such $Q = \pm 1/3$ configurations. For a given $Q_n = \pm 1/3$ the number of configurations $Z_{1,N}$ differs from the number of ground states, Z_N by some numerical factor, w_1. We estimate the factor w_1 the same naive way as we estimated the number of ground states, i. e. we assume that chiralities ± 1 have equal and independent probabilities. This yields $w_1 \approx 21/22$. The precision of this estimate is again of order 1/6 and we set in follows $w_1 = 1$. Denoting the long-wavelength part of $J(\mathbf{R})$ as $3K\Psi(\mathbf{R})$, where $K = \beta/12$, we arrive at the long-distance effective action in the standard form:

$$Z = \int \mathrm{D}\Psi(\mathbf{r}) \times \qquad (10)$$

$$\times \exp\left\{-\int d^2\mathbf{r}\left[\frac{\sqrt{3}K}{2}(\nabla\Psi)^2 - ha^{-2}\cos(2\pi K\Psi)\right]\right\},$$

where $h = 2e^{-K\pi^2/2} = 2e^{-\beta\pi^2/24}$ and $a = |\mathbf{a}|$. At the BKT transition temperature, this is a small field, that allows one to use the perturbative renormalization group approach [7]. The BKT transition occurs at the temperature where the field h becomes relevant. For the hexagonal lattice we get $\sqrt{3}/2K_c = \pi/2$, i. e.

$$T_c/\kappa S^2 = \sqrt{3}\pi/72 = 0.0756. \qquad (11)$$

We neglected nonlinear terms which can slightly renormalize the stiffness constant. This effect on T_c is small because of to the smallness of $T_c/\kappa S^2$ (see also [8]).

The existence of a new set of variables, chiralities, qualitatively changes the spin correlation function compared to that in unfrustrated XY magnets. Returning to the initial formulation of the problem (2), we consider the correlation functions $\mathcal{K}_j(r_0) = \langle \exp\left(i[\theta(0) - \theta(\mathbf{r}_0)] \cdot j\right)\rangle$. In terms of the integer-valued variables, $n(\mathbf{r}, \mathbf{a})$, we arrive at an expression that differs from (4), only by arguments of the δ-functions. Namely, for sites 0 and $\mathbf{r_0}$ we get

$$\sum_{\mathbf{a}} n(\mathbf{0}, \mathbf{a}) = -\sum_{\mathbf{a}} n(\mathbf{r}_0, \mathbf{a}) = j, \qquad (12)$$

instead of the conservation condition (5). This condition is equivalent to a pattern of currents which is a superposition of currents $J(\mathbf{R}_h)$, that flow in the kagomé lattice and obey the condition (5), and a current j which takes a whole number value and which is created in the point $\mathbf{0}$ and is annihilated in the point $\mathbf{r}_0$. Thus, the correlation function $\mathcal{K}_j(r_0)$ has the form

$$\mathcal{K}_j(r_0) = \frac{1}{Z(\beta)} \sum_{\{J(\mathbf{R})\}} \prod_{(\mathbf{R}\neq\mathbf{R}^*, \mathbf{A}\neq\mathbf{A}^*)} \times \qquad (13)$$

$$\times I_{J(\mathbf{R}+\mathbf{A})+J(\mathbf{R})}(-\beta) \prod_{(\mathbf{R}^*, \mathbf{A}^*)} I_{J(\mathbf{R}^*+\mathbf{A}^*)+J(\mathbf{R}^*)+j}(-\beta).$$

Here $(\mathbf{R}^*, \mathbf{A}^*)$ are sites and vectors of the dual lattice such that $\mathbf{A}^*$ crosses the path $(\mathbf{0}, \mathbf{r}_0)$ on the initial kagomé lattice. Integrating over currents in the triangles in (13) we get: $\mathcal{K}_j(r_0) = Z_j(\beta, r_0)/Z(\beta)$ where $Z(\beta)$ is given by Eq. (8) and $Z_j(\beta, r_0)$ differs from $Z(\beta)$ by the additional contribution from the current j running along the path $(\mathbf{0}, \mathbf{r}_0)$.

The contribution of $Q \neq 0$-configurations (vortex) to the large r_0 asymptotics of the spin correlation function $\mathcal{K}_j(r_0)$ below the BKT transition point is negligible because the renormalization group flow at $T < T_c$ yields that the effective constant h in (10) is equal to zero. The main difference between our $\mathcal{K}_j(r_0)$ and the usual (unfrustrated) case is in the factor

$$\exp(2\pi i \sum_{\mathbf{R}_t^*} \frac{\sigma(\mathbf{R}_t^*)}{3} \cdot j) \qquad (14)$$

averaged over chiralities. For simplicity we consider the case when the shortest walk on lattice sites between points 0 and r_0 is a straight line. In this case, r_0/a is the number of bounds along this walk, where a is the kagomé lattice constant. Neglecting constrains on chiralities of triangles as we did before we immediately get a factor $(\cos 2\pi/3)^{r_0/a} = (-1)^{r_0/a}2^{-r_0/a}$ in the correlation function when j is not a multiple of 3. The integration over $J(\mathbf{R}_h)$ in the $r_0 \to \infty$ limit can be done in the spin-wave approximation and gives the well-known result [1]. Thus, in the low-temperature phase $T \leq T_c$ in the long-distance limit $r_0/a \gg 1$ the spin correlation function reads

$$\mathcal{K}_j(r_0) \propto (-1)^{r_0/a}2^{-r_0/a}(r_0/a)^{-j^2T/36T_c}, \quad j \neq 3, 6, 9 \dots \tag{15}$$

It decays exponentially with distance. Note that the statement about exponential decay of the spin-spin correlators does not depend on the approximations made here. It follows from finitness of the correlation length of the chiralities field. The true order parameter of the BKT transition is the cubed spin [4], $\eta(\mathbf{r}) = \exp(3i\theta(\mathbf{r}))$. The correlation function of this order parameter at $T < T_c$ decays as a power of distance

$$\mathcal{K}_3(r_0) = < \eta(0)\eta^*(\mathbf{r}) > \sim (r_0/a)^{-T/4T_c}. \tag{16}$$

The result for T_c is in agreement with Monte-Carlo simulations of the BKT transition in the kagomé antiferromagnet [6] and with the recent independent calculations [11]. (Note that the preprint version of the present paper was published before [12]). In the paper [11] it is shown that next-to-nearest neighbors exchange interaction on kagome lattice can remove the degeneracy of the ground state. However, the spin-spin interaction induced by thermal spin waves cannot play the same role. Indeed, in the case of nearest neighbors interaction considered here spots of $\sigma(\mathbf{R})$ with changed signs have finite entropy at $T \to 0$. Their contribution to the free energy and correlators dominates and the effect of interaction induced by spin waves considered in [11] are negligible at small temperatures.

This research was partially supported by grants # NPF000 and # NPF300 from the International Science Foundation and the Russian Government, and by the Russian Foundation for Fundamental Research (grant # 96-02-19125a). We are pleased to thank P. Coleman and C. Henley for useful remarks. We are grateful to M. V. Feigelman for stimulating remark.

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